Stark ionisation of hydrogen in the n=2 level. Asymmetry in the final transverse velocity

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Stark Ionisation of hydrogen in the n=2 level. Asymmetry in the final transverse velocity[1]

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Abstract. The effect of orbital momentum in the strong field ionization of a hydrogen atom is considered. When the atom is in the 2P state an asymmetrical distribution in the transverse velocity $\mathbf{v}_\mathrm{T}$, similar to the Collins effect in quark fragmentation, is predicted : $\langle \mathbf{v}_\mathrm{T} \rangle$ points in the direction of $\mathbf{E} \times \langle \mathbf{L} \rangle$. However, the Stark efffect produces oscillations of the average orbital angular momentum $\langle \mathbf{L}_\mathrm{T} \rangle$, therefore of $\langle \mathbf{v}_\mathrm{T} \rangle$.

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INTRODUCTION

The electronic states of an atom in a uniform electric field are modified by the Stark effect. If the field is strong enough, ionization of the atom eventually occurs due to the tunnel effect. The probability of ionisation per unit of time is given in Ref.[1] for an hydrogen atom in the ground state.

In the case where the electron is initially in a state of orbital angular momentum $l \neq 0$ with $\langle \mathbf{L} \rangle$ perpendicular to the field $\mathbf{E}$, it was expected [2] that the transverse velocity of the extracted electron is in average in the direction of $\mathbf{E} \times \langle \mathbf{L} \rangle$. This azimuthal asymmetry, pictured in Fig.1a, is analogous to the Collins effect in quark fragmentation [3], for which a *string* + $^3\mathrm{P}_0$ mechanism is represented in Fig.1b.

In this work we will study quantitatively the Collins-like effect for a hydrogen atom initially in the state $n = 2$, $l = 1$, $L_y = \pm 1$. A complication arises from the fact that, for a pure Coulomb potential, the *linear* Stark effect mixes the S wave and the $L_z = 0$, P-wave maximally. Since the $L_y = \pm 1$, P-waves have nonvanishing projections on the $L_z = 0$, P-wave, they are affected by the linear Stark effect as well. In particular, oscillations between different L_y states are expected to occur.

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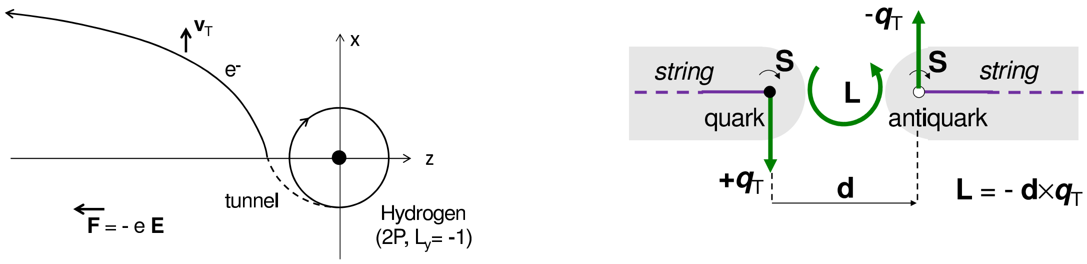

(a) (b)

FIGURE 1. **(a)** Classical motion of the electron extracted form the hydrogen atom by a strong field **E**, when the electron is initally in a $L_y = -1$ state. **(b)** The string + ^{3}P$_0$ mechanism correlating the tranverse momentum and the transverse polarization of a quark created in string decay [2].

SCHRÖDINGER EQUATION IN PARABOLIC COORDINATES

The atom is in the constant electric field $\mathbf{E} = -\mathbf{F}/e = (0,0,F/e)$. As in ref. [1] we introduce the parabolic coordinates

$$\xi = r+z \qquad \eta = r-z, \qquad \varphi = \arg(x+iy) \tag{1}$$

and look for wave functions of the form

$$\Phi = N\frac{\chi_1}{\sqrt{\xi}}(\xi)\,\frac{\chi_2}{\sqrt{\eta}}(\eta)\,e^{im\varphi}. \tag{2}$$

Using the atomic units $\hbar\,(m_e\alpha c)^{-1} = 0.0529$ nm for lengths and $m_e\alpha^2c^2 = 27,2$ eV for energies, χ_1 and χ_2 verify the separate equations

$$\frac{\partial^2\chi_1}{\partial\xi^2} + \left[\frac{1}{2}E + \frac{1-\beta}{\xi} - \frac{m^2-1}{4\xi^2} - \frac{1}{4}F\xi\right]\chi_1 = 0 \tag{3a}$$

$$\frac{\partial^2\chi_2}{\partial\eta^2} + \left[\frac{1}{2}E + \frac{\beta}{\eta} - \frac{m^2-1}{4\eta^2} + \frac{1}{4}F\eta\right]\chi_2 = 0. \tag{3b}$$

UNPERTURBED WAVE FUNCTIONS OF THE LEVEL N = 2

We present here the wave functions Φ_{nlm} in the absence of external field for n = 2 and various combinations of them which will be used later, in spherical or parabolic coordinates.

- ***States*** $m \equiv L_z = 0$.

$$\begin{aligned}\Phi_0 &\equiv \Phi_{200} = (4\sqrt{2\pi})^{-1}\,(2-r)\;e^{-r/2}\\ \Phi_Z &\equiv \Phi_{210} = (4\sqrt{2\pi})^{-1}\,z\,e^{-r/2}.\end{aligned}$$

$$\Phi_{Z+} = \frac{\Phi_0+\Phi_Z}{\sqrt{2}} = \frac{1}{8\sqrt{\pi}}e^{-\xi/4}\,(2-\eta)\,e^{-\eta/4},\ \text{with } \beta = 3/4, \tag{4}$$

$$\Phi_{Z-} = \frac{\Phi_0 - \Phi_Z}{\sqrt{2}} = \frac{1}{8\sqrt{\pi}} (2-\xi)\, e^{-\xi/4} e^{-\eta/4}, \text{ with } \beta = 1/4 \tag{5}$$

- ***States*** $m \equiv L_z = \pm 1$.

$$\Phi_{Lz\pm} = \mp \frac{1}{8\sqrt{\pi}} \sqrt{\xi}\; e^{-\xi/4}\; \sqrt{\eta}\; e^{-\eta/4}\; \exp(\pm i\phi), \text{ with } \beta = 1/2 \tag{6}$$

- ***The P-state of*** $L_x = 0$. Combining the $\Phi_{21\pm1}$ states we define

$$\Phi_X \equiv \Phi_{21,\, Lx=0} = \frac{-\Phi_{211} + \Phi_{21-1}}{\sqrt{2}} = \frac{1}{4\sqrt{2\pi}} \sqrt{\eta} e^{-\eta/4} \sqrt{\xi} e^{-\xi/2} \cos\phi. \tag{7}$$

- ***The states of*** L_y**=**± 1. To highlight the asymmetry in $\mathbf{F} \times \mathbf{L}$, we study the strong field ionization of the $L_y = \pm 1$ eigenstates

$$\Phi_{Ly\pm} = \frac{\Phi_Z \pm i\Phi_X}{\sqrt{2}} = \frac{1}{8\sqrt{\pi}} (z \pm ix)\; e^{-r/2}. \tag{8}$$

These two states are not separable in parabolic coordinates but we can decompose them along the separable states:

$$\Phi_{Ly\pm} = \frac{1}{2}\Phi_+ - \frac{1}{2}\Phi_- \pm \frac{i}{\sqrt{2}}\Phi_X. \tag{9}$$

LINEAR STARK EFFECT

When the external field F is present the states Φ_0 and Φ_Z are no longer eigenstates of the *Stark hamiltonian* $H_0 + Fz$. To lowest order in F the new eigenstates are the Stark states Φ_{Z+} and Φ_{Z-} given by Eqs.(4,5). The $m = \pm 1$ states remain eigenstates. Denoting by $\overline{E} = -1/8$ the unperturbed energy for $n = 2$, the new energies are:

$$\begin{array}{ll} \overline{E} & \text{for} \quad \Phi_{Lz\pm}\,, \Phi_X\,, \\ \overline{E} \mp 3F & \text{for} \quad \Phi_{Z\pm}\,. \end{array}$$

If one puts the atom at some time in a state which is not an eigenstate of $H_0 + F_z$, it will oscillate between the old eigenstates. For instance if the electron is in state (8) at $t = 0$, its wave function at $t \neq 0$ is

$$\Psi(t) = e^{-i\overline{E}t} \left(e^{+3iFt}\, \Phi_+/2 - e^{-3iFt}\, \Phi_-/2 \pm \Phi_X/\sqrt{2} \right). \tag{10}$$

Using (4), (5), (7) and (8), we obtain the two equivalent expressions

$$\Psi(t) = 2^{-1/2} e^{-i\overline{E}t} \left[\cos(3Ft)\, \Phi_Z + i \sin(3Ft)\, \Phi_0 \pm i\Phi_X\right], \tag{11}$$

$$\Psi(t) = e^{-i\overline{E}t} \left[\cos^2\left(\frac{3Ft}{2}\right) \Phi_{Ly\pm} - \sin^2\left(\frac{3Ft}{2}\right) \Phi_{Ly\mp} + \frac{i}{\sqrt{2}} \sin(3Ft)\, \Phi_0 \right], \tag{12}$$

which display oscillations.

TUNNEL EFFECT ON STARK PROPER STATES

To all order in F the states (4-7) are not stable due to the tunnel effect. The exact wave function has oscillatory asymptotic part which is the wave of the escaping electron. Using the method of Ref. [1] we obtain the following asymptotic forms at $\eta \gg \overline{\eta}_1 = |2\overline{E}|/F$:

$$\Phi_X = \frac{\sqrt{\xi}e^{-\xi/4}}{8F\sqrt{2\eta\pi p(\eta)}} \exp\left(-\frac{1}{24F} + \frac{i\sqrt{F}}{3}(\eta - \overline{\eta}_1)^{3/2} + \frac{5i\pi}{4}\right)\cos\phi\,, \tag{13}$$

$$\Phi_{Z+} = \frac{-e^{-\xi/4}}{16\sqrt{\pi\eta p(\eta)F^3}} \exp\left(-\frac{1}{24F} - \frac{3}{2} + \frac{i\sqrt{F}}{3}(\eta - \overline{\eta}_1)^{3/2} - 6i\overline{p}(\eta) + \frac{7i\pi}{4}\right) \tag{14}$$

$$\Phi_{Z-} = \frac{(2-\xi)\,e^{-\xi/4}}{16\sqrt{\eta\pi p(\eta)F}} \exp\left(-\frac{1}{24F} + \frac{3}{2} + \frac{i\sqrt{F}}{3}(\eta - \overline{\eta}_1)^{3/2} + 6i\overline{p}(\eta) + \frac{i3\pi}{4}\right), \tag{15}$$

where $\overline{p}(\eta) \simeq \frac{1}{2}\sqrt{F\,(\eta - \overline{\eta}_1)}$ is the local quasi-classical momentum of the Φ_X wave. From these expressions we obtain the corresponding ionization rates [4] :

$$\begin{aligned} 1/\tau_X &= 2^{-5}F^{-2}\exp[-1/(12F)]\,, && \text{(16a)}\\ 1/\tau_{Z+} &= 2^{-6}F^{-3}\exp[-1/(12F) - 3]\,, && \text{(16b)}\\ 1/\tau_{Z-} &= 2^{-4}F^{-1}\exp[-1/(12F) + 3]\,. && \text{(16c)} \end{aligned}$$

For the superposition (10),

$$\Psi(t) = \frac{iQ(\tau,\xi\,\varphi)}{32\sqrt{\pi\eta p(\eta)F^3}} \exp\left(-\frac{1}{24F} - \frac{3}{2} + \frac{i\sqrt{F}}{3}(\eta - \overline{\eta}_1)^{\frac{3}{2}} - i\overline{E}t + i\pi/4\right), \tag{17}$$

where

$$Q(\tau,\xi\,\varphi) = \left[e^{3iF\tau} - (2-\xi)\,ge^{-3iF\tau} \mp 2\sqrt{\xi g}\cos\varphi\right]e^{-\xi/4}\,, \tag{18}$$

$g \equiv \exp(-3)F$ and $\tau \equiv t - \sqrt{(\eta - \overline{\eta}_1)/F} \simeq t - \sqrt{2|z - \overline{z}_1|/F}$.

Using the approximation $\eta = (x^2+y^2)/\xi \simeq 2|z|$, one can see that $|\Psi|^2$ behaves like a classical density of electrons falling freely in the uniform force field $\mathbf{F}$. Each such electron leaves the atom at time τ and follows a parabolic motion of definite ξ and φ:

$$(x,y) = \sqrt{F\xi}\,(t-\tau)\,(\cos\varphi, \sin\varphi), \quad |z| = F(t-\tau)^2/2\,. \tag{19}$$

The average transverse position at fixed z and t is given by $\langle y\rangle = 0$ and

$$\langle x(t,z)\rangle = \frac{\int xdxdy\,|Q|^2}{\int dxdy\,|Q|^2} \simeq \mp 4e^{-3/2}\sqrt{2|z|F}\cos\left(3Ft - 3\sqrt{2F(z-\overline{z}_1)}\right)\,. \tag{20}$$

For fixed τ it corresponds to a parabolic motion at constant tranverse velocity $v_x = \mp 4e^{-3/2}F\cos(3F\tau)$. This confirms the oscillating Collins-like effect. The dorsal line $\langle x(t,z)\rangle$ of the electron density, shown in Fig.2, undulates like a snake.

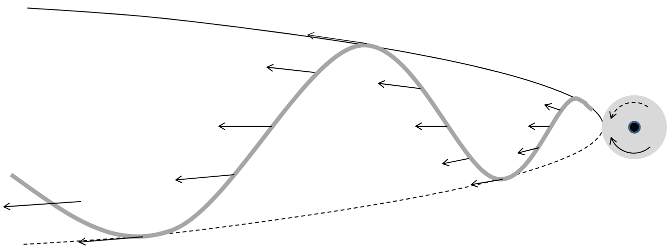

FIGURE 2. Curve (in grey) giving the mean transverse position of the escaping electron as a function of z at a given time. As time grows, the undulations move to the left. The axes are the same as in Fig.1a.

DISCUSSION

At most, $\langle x \rangle$ is smaller than the root mean square value $\langle x^2 \rangle^{1/2} = \sqrt{2|z|}$ by the factor $e^{-3/2} F^{1/2}$. It means that the memory of the initial angular momentum is lost when F is too small, *i.e.,* when the tunnel is too long.

The 2P state of the hydrogen atom has a finite lifetime with respect to the radiative transition to the 1S state. If no external field is present, the radiative decay rate is given by

$$\tau_{\rm rad}^{-1} = (2/3)^8 \, mc^2 \alpha^5 / \hbar$$

$= 1.5\, 10^{-8}$ in atomic units. In order to obtain the tunneling ionization, the field $\mathbf{E}$ must not be too weak, otherwise the radiative transition will take place before.

The atomic unit of field is $m(\alpha c)^2/a_0 \simeq 514$ volt/nm. The highest macroscopic static electric fields which can be obtained is of the order of 3 volt/nm $\simeq$ 1/171 atomic units. The corresponding factor $\exp(-1/12F)$ of tunneling is then $\exp(-14)$. This seems to make the experiment difficult. Perhaps one could find an atom excited in the P-wave which is easier to ionise than the $n = 2$ hydrogen atom, so that the Collins-like effect could be experimentally observed. But in this case the Stark effect will be quadratic, hence less important, and one should have no oscillation.

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